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Modeling and Optimal Design of a Chemical Vapor Deposition Reactor*

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Abstract

In this paper the flow dynamics of a homogeneous gas inside a vertical, cylindrical reactor is modeled with a commercially available computational fluid dynamics code. The transport processes in chemical vapor deposition are described by conservation of mass, momentum, energy, and mass transfer equations. Navier-Stokes equations for a Newtonian fluid and laminar flow are used to describe the momentum conservation. Buoyancy effect is included in the model through the gravitational term in the momentum equation. Thermal (Soret) effect will also included in the model to account for binary diffusion in the presence of large temperature gradients typical of chemical vapor deposition (CVD) process. Results of a 2-D, steady, axi-symmetrical flow are presented using a finite element method with non-uniform cartesian meshes. We also provide some discussions on the formulation of the optimal reactor design problem for CVD.

1. Introduction

Chemical vapor deposition is an industrial process used to produce thin films in microelectronic devices (e.g. transistors, integrated circuits, super-conducting devices). This process uses chemically reacting vapors to create an epitaxial (thin) film. One of the common CVD processes is the the deposition of extremely-pure epitaxial films of compound semiconductors for optoelectronic and high-speed electronic devices. Use of the epitaxial film for these devices requires uniformity of the thickness and precise control of composition of the layers grown. These, in turn, depend strongly on gas flow dynamics in the deposition chamber (reactor). The purpose of this project is to create an optimized design of the reactor chamber with a view to increased purity and uniformity of the deposition layer. We also study the use of active controls with the same goal of growing better epitaxial layers.

Deposition at atmospheric or slightly reduced pressures (≈ 0.1 atm) is desirable for high growth rates, making the control of uniformity very difficult. Thus, much attention has been given to the area of modeling gas flow in the vertical and horizontal CVD reactors through numerical simulation studies. For example, Black et al. [1] have presented a 2-D model of CVD growth of GaAs in a horizontal reactor and validated their results against experimental data for in the low pressure high-flow rate regimes. Also, Ouazzani et al. [9] investigated a 3-D model of horizontal CVD and compared their results with experimental data. One of their primary findings was that for light gases, thermal (Soret) diffusion cannot be neglected in the modeling. Their models also predicted that Soret diffusion increases the uniformity of growth process. CVD and related thin film deposition processes are reviewed in a number of books and articles (see e.g. [3] and the references given therein). A review of the transport phenomena and chemistry involved in CVD can be found in [7], [5].

In recent years there has been increased inter-

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est in control problems arising in fluid flow systems. However, most of the progress so far has been limited to numerical experimental investigations. For example in the area of boundary layer separation control, several methods have been developed experimentally to provide various effective results of flow control including a moving surface, and suction or injection of a gas (see e.g. [6]). We will use analytic methods to determine effective controls to be used in the context of CVD, such as the method demonstrated by Ito et al. [4]. They formulated and solved (computationally) the control of recirculation in a steady-state problem for two flows, namely, the driven cavity flow, and a flow over a backstep where there is a sudden expansion. Other contributions in the analytical or numerical approach of fluid flow control are presented in [8, 10, 11, 2]. In formulating the control problem a crucial step is to find a suitable *cost functional* that is relevant to the physics of the flow. The cost functional is a quantification of the goals we want to achieve. For example, the integral of the magnitude of the vorticity would be a quantification of the goal to achieve laminar flow. The cost function for this application is described below.

2. Problem Specification

We will use a reactor with a configuration designed to reduce fluctuations in flow conditions. Such fluctuations can arise, for example, from buoyancy effects and from irregular geometries. We minimize the loss of symmetry by choosing a cylindrical tube, and minimize non-axisymmetric buoyancy effects by aligning the gravitational vector **g** with the axis of symmetry and using upwards flow of gas in the CVD reactor. This orientation will protect the downwards facing substrate from particulates that may settle on the surface and cause inhomogeneous growth conditions across the wafer. The configuration for the 2-dimensional simulation is shown in Fig. 1. This is for comparison with the planned closed-tube reactor experimental setup depicted in Fig. 2.

3. Model

The mathematical model for the transport phenomena involved in the CVD process couples

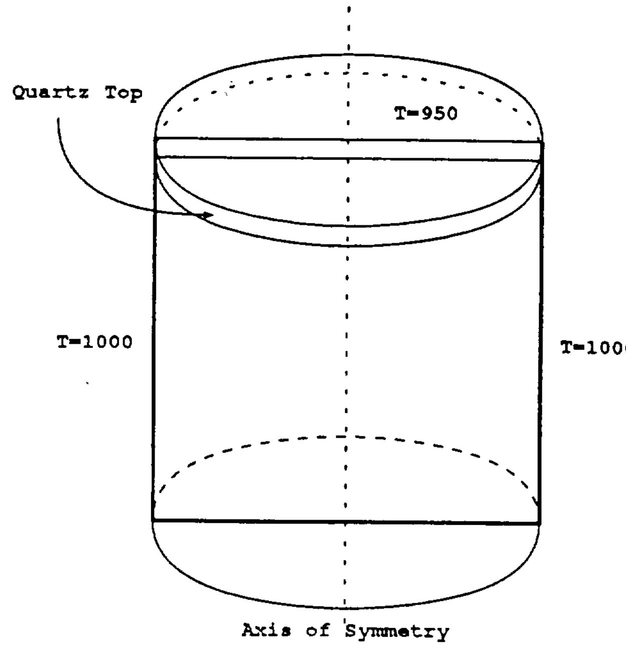

Figure 1: Simplified geometry for numerical experiments

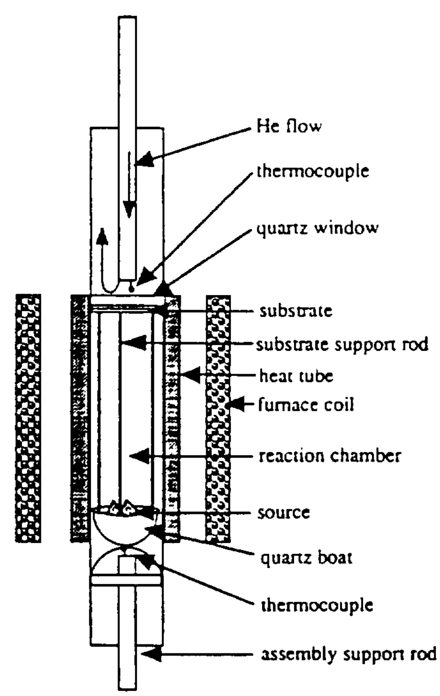

Figure 2: Actual Reactor Configuration

the usual gasdynamic equations (conservation of mass, momentum and energy) with an equation for the effects of species diffusion. For example, if we assume a binary mixture of gases indicated by the subscripts a and b, the species diffusion equation would be

$$\frac{\partial(\rho W_b)}{\partial t} + \frac{\partial(\rho u W_b)}{\partial x} + \frac{\partial(\rho v W_b)}{\partial y} + \frac{\partial(\rho w W_b)}{\partial z} =$$

$$\frac{\partial}{\partial x}\left[\rho D_{ab}\frac{\partial W_b}{\partial x}\right] + \frac{\partial}{\partial y}\left[\rho D_{ab}\frac{\partial W_b}{\partial y}\right] + \frac{\partial}{\partial z}\left[\rho D_{ab}\frac{\partial W_b}{\partial z}\right]$$

$$+\frac{\partial}{\partial x}\left[\rho D_{ab}\alpha_T W_a W_b \frac{\partial \log T}{\partial x}\right]$$

$$+\frac{\partial}{\partial y}\left[\rho D_{ab}\alpha_T W_a W_b \frac{\partial \log T}{\partial y}\right]$$

$$+\frac{\partial}{\partial z}\left[\rho D_{ab}\alpha_T W_a W_b \frac{\partial \log T}{\partial z}\right]$$

In this equation, ρ is the density of carrier gas, u, v and w are the velocity components in the x, y and z direction respectively, W_a is the mass fraction of carrier gas, W_b is the mass fraction of reactant, D_{ab} is the diffusion constant of reactant in carrier gas, α_T is the thermal diffusion factor, and T is the temperature. Using these equations for the gasdynamics, the deposition process is modeled through special boundary conditions at the substrate. This is a topic of current study.

We note that gravity enters into the transport model through the momentum equation, and thermal (Soret) diffusion is modeled in the species equation by the terms

$$\frac{\partial}{\partial \xi}\left[\rho D_{ab}\alpha_T W_a W_b \frac{\partial \log T}{\partial \xi}\right]$$

where ξ stands for x, y, or z. This is the separation of species of different mass or size due to thermal gradients.

4. Numerical Simulations

In our first case study, we consider a two-dimensional axi-symmetric steady flow of a homogeneous gas with the properties of air at 20 atmospheres. The mesh density used in the computation is depicted in Fig. 3. The top wall is fused quartz with thickness of 2 mm. The dimension of the tube is 5cm by 5cm. We used no-slip boundary conditions everywhere (i.e. the velocity is zero). The temperature is fixed at 950°C at the top of the fused quartz wall and 1000°C otherwise. This simulation is designed to provide insight into the bulk flow. Modeling of the deposition process itself is a topic of current study.

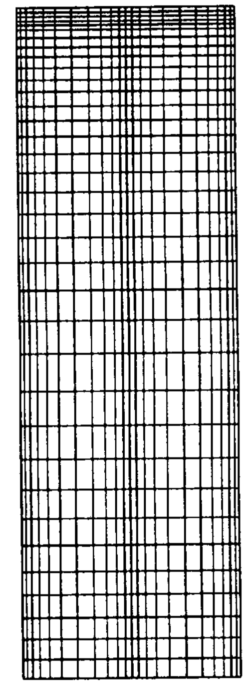

Figure 3: Mesh for 2-D Simulation

The problem is solved using the finite element code FIDAP on the Cray Y-MP. The CPU time for a typical simulation is 10 sec. The velocity field (see Fig. 4) contains recirculating cells. When the material in the recirculating regions cannot exit these regions except by diffusion, these vortices in the CVD reactor will adversely effect the film uniformity. We remark that buoyancy driven recirculating cells appeared in the atmospheric pressure (open tube) simulations calculated by Black et al. [1].

5. Optimization of Reactor and Active Control of Flow

The first stage of this project is the creation of an optimized reactor chamber design. This will be followed by studying techniques to actively control the fluid fluid flow. When formulating control and/or optimization problems for

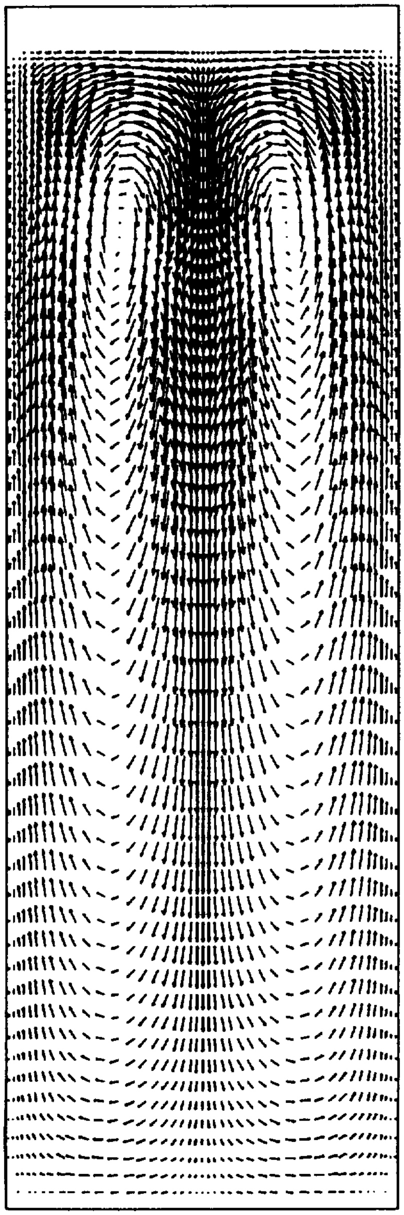

Figure 4: Velocity field

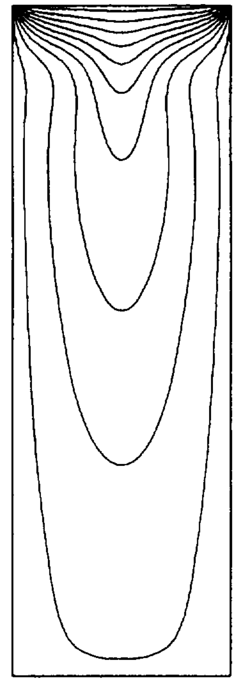

Figure 5: Temperature contours

the flow in CVD reactors, a very important step is the derivation of a suitable cost functional relevant to the physics of the flow. Both the reactor chamber design and control of fluid flow share the ultimate goal of uniformity of the epitaxial layer; however, measuring the uniformity in the computational setting may not be possible (due to simplifications required to formulate the model of the deposition process). Thus, the cost functional must be formulated as depending on other quantities. One candidate cost functional corresponds to matching the velocity field inside the CVD reactor with a desired field given by $\vec{u}^d$. This cost functional is

$$\int_0^T \int_\Omega \|\nabla(\vec{u} - \vec{u}^d)\|^2 \, dx \, dt,$$

where $\Omega \subset R^n$, $n = 2$ or 3, denote the geometry of the reactor, $\vec{u}$ is the velocity vector of the flow. Another cost functional corresponds to the total vorticity in the flow given by

$$\int_0^T \int_\Omega \|\nabla \times \vec{u}\|^2 \, dx \, dt.$$

This cost is motivated by the fact that flows with small vorticity should contain little recirculation.

Minimizing the cost functional for active control of the fluid flow can exploit the possibility of modifying the following experimental parameters:

1. modifying the temperature profile at the top of the reactor,
2. rotation of the reactor chamber,
3. and/or slight modification of the orientation of the reactor chamber with respect to the gravity vector.

Optimal reactor design can utilize the above parameters; however, the design is expected to depend primarily on the following parameters (refer to Fig. 2):

1. shape of the quartz top (e.g. convex up, down, or a combination),
2. height of the reactor chamber,
3. and shape of the bottom of the reactor chamber respect to the gravity vector.

We expect to show the feasibility of the above formulation of control problems by developing computational algorithms for optimal solutions for specific CVD processes of practical importance.

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